Excited State Evolution towards Ligand Loss and Ligand Chelation at Group 6 Metal Carbonyl Centres

Jennifer C. Manton,[a] Saeed Amirjalayer,[b] Anthony Coleman,[a] Suzanne McMahon,[a] Emma C. Harvey,[a] Gregory M. Greetham,[c] Ian P. Clark,[c] Wybren Jan Buma,[b] Sander Woutersen,[b] Mary T. Pryce,[a] Conor Long[a*]

Supporting Information

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Analysis of excited states and orbital compositions

(eta-6-Benzophenone)Cr(CO)3

Molecule: C16H10CrO4
 Details: #p b3lyp/Tzvp Geom=Check SCF=Tight Pop=Full IOp(3/33=1)
 Source file: benzphenonePt0AOMix.log
 Population analysis: MPA
  473 orbitals(473 canonical) 81 alpha + 81 beta electrons
 Number of fragments: 3
 Fragment 1 (24 atoms, 326 orbitals): Benzophenone
 Fragment 2 (6 atoms, 114 orbitals): CO Ligands
 Fragment 3 (1 atoms, 33 orbitals): Cr

 COMPOSITIONS OF MOLECULAR ORBITALS (GROSS CONTRIBUTIONS, %)
 AND OVERLAP POPULATIONS (OP) BETWEEN FRAGMENTS

Alpha MO:	71	72	73	74	75	76	77	78	79	80
	HOMO-10	HOMO-9	HOMO-8	HOMO-7	HOMO-6	HOMO-5	HOMO-4	HOMO-3	HOMO-2	HOMO-1
Energy(eV):	-10.45	-10.30	-10.00	-9.13	-8.97	-7.78	-7.61	-7.36	-6.19	-6.01
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	97.87	99.07	99.62	85.21	86.90	99.46	99.92	99.67	3.84	15.14
FRAG# 2:	1.09	0.47	0.15	2.12	1.92	0.09	0.02	0.04	24.06	23.77
FRAG# 3:	1.04	0.46	0.23	12.68	11.18	0.46	0.07	0.28	72.10	61.10
OP(1 & 2)	-0.004	-0.001	0.000	-0.002	0.002	0.000	0.000	-0.001	0.006	0.014
OP(1 & 3)	0.004	0.002	0.001	0.094	0.079	0.001	-0.001	0.001	-0.075	0.030
OP(2 & 3)	0.002	0.000	0.000	-0.004	-0.004	0.000	0.000	0.000	0.085	0.081

Alpha MO:	81	82	83	84	85	86	87	88	89	90
	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4	LUMO+5	LUMO+6	LUMO+7	LUMO+8
Energy(eV):	-5.99	-2.47	-1.41	-1.21	-0.88	-0.56	-0.53	-0.36	0.20	0.30
Symmetry:	na	na	na	na	na	na	na	na	na	na
FRAG# 1:	20.44	84.40	83.68	89.48	96.48	17.22	14.54	14.76	50.85	6.78
FRAG# 2:	22.01	7.43	11.58	7.39	2.30	39.36	43.44	54.99	11.16	57.43
FRAG# 3:	57.55	8.17	4.74	3.13	1.22	43.42	42.01	30.25	37.99	35.79
OP(1 & 2)	0.013	-0.036	-0.113	-0.090	-0.008	-0.273	-0.262	-0.510	0.269	0.211
OP(1 & 3)	0.036	-0.106	-0.058	-0.045	-0.014	-0.494	-0.393	-0.722	-1.124	-0.499
OP(2 & 3)	0.075	0.039	-0.004	-0.022	-0.001	0.094	0.126	0.039	-1.572	-1.051

Excitation energies and oscillator strengths:

 Excited State 1: Singlet-A 2.5207 eV 491.86 nm f=0.0007 <S**2>=0.000
  80 -> 82 0.68655
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) = -1961.39734728
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State 2: Singlet-A 2.6906 eV 460.80 nm f=0.0001 <S**2>=0.000
  79 -> 82 0.68920

 Excited State 3: Singlet-A 2.8326 eV 437.71 nm f=0.0666 <S**2>=0.000
  80 -> 83 0.21390
  81 -> 82 0.65005

 Excited State 4: Singlet-A 3.4022 eV 364.42 nm f=0.0002 <S**2>=0.000
  79 -> 84 -0.13267
  79 -> 86 -0.29986
  79 -> 87 0.11347
  80 -> 86 -0.12229
  81 -> 83 0.47595
  81 -> 84 0.18815
  81 -> 86 0.16583
  81 -> 87 0.19062

 Excited State 5: Singlet-A 3.4463 eV 359.76 nm f=0.0012 <S**2>=0.000
  79 -> 83 0.19387
  79 -> 84 0.14587
  79 -> 86 0.29752
  79 -> 87 0.35630
  79 -> 94 -0.15815
  80 -> 83 0.12305
  80 -> 86 0.11838
  81 -> 83 0.28892
  81 -> 86 -0.14947

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Excited State   6:      Singlet-A      3.4533 eV  359.03 nm  f=0.0007  <S**2>=0.000
     79 -> 84       -0.14347
     79 -> 86       -0.28850
     79 -> 87        0.21465
     80 -> 84        0.21471
     80 -> 86        0.41098
     80 -> 87       -0.16558
     81 -> 87       -0.18188

Excited State   7:      Singlet-A      3.5535 eV  348.91 nm  f=0.0011  <S**2>=0.000
     79 -> 83        0.12029
     79 -> 87        0.30706
     79 -> 94       -0.13376
     80 -> 86       -0.14962
     81 -> 83       -0.33790
     81 -> 84       -0.11313
     81 -> 87        0.37688
     81 -> 94       -0.15733

Excited State   8:      Singlet-A      3.5822 eV  346.11 nm  f=0.0005  <S**2>=0.000
     79 -> 83        0.14542
     79 -> 88        0.15342
     80 -> 83       -0.14051
     80 -> 86        0.13203
     80 -> 87        0.39481
     80 -> 94       -0.13647
     81 -> 83       -0.12785
     81 -> 84        0.16663
     81 -> 86        0.38172
     81 -> 87       -0.10333

Excited State   9:      Singlet-A      3.6388 eV  340.73 nm  f=0.0004  <S**2>=0.000
     79 -> 83        0.60751
     79 -> 84        0.12473
     79 -> 87       -0.12438
     80 -> 87       -0.19170

Excited State  10:      Singlet-A      3.6487 eV  339.80 nm  f=0.0039  <S**2>=0.000
     76 -> 82       -0.36329
     78 -> 82        0.57793
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(eta-6-AllylBenzene)Cr(CO)3


 Molecule:    C12H10CrO3
 Details: #P b3lyp/Tzvp Pop=Full SCF=Tight IOp(3/33=1) Guess=Read Geom=Check
 Source file: AllylB3LYPTzvpAOMix.log
 Population analysis: MPA
  378 orbitals(  378 canonical)  65 alpha +  65 beta electrons
 Number of fragments:    3
 Fragment   1 (   1 atoms,   33 orbitals): Cr
 Fragment   2 (   6 atoms,  114 orbitals): (CO)3
 Fragment   3 (  19 atoms,  231 orbitals): Allylbenzene

   Alpha MO:      61      62      63      64      65      66      67      68      69      70
              HOMO-4  HOMO-3  HOMO-2  HOMO-1    HOMO    LUMO  LUMO+1  LUMO+2  LUMO+3  LUMO+4
 Energy(eV):   -8.68   -7.72   -5.98   -5.77   -5.76   -1.27   -1.20   -0.43   -0.38   -0.35
   Symmetry:     na      na      na      na      na      na      na      na      na      na
==========================================================================================
 FRAG#    1:   11.03    0.59   71.61   59.84   60.73    5.63    5.17   18.70   40.15   31.50
 FRAG#    2:    1.94    0.08   25.16   24.48   24.87   11.63   11.26   13.51   44.38   38.76
 FRAG#    3:   87.03   99.32    3.24   15.69   14.40   82.74   83.58   67.79   15.47   29.74
OP( 1 &  2 )  -0.005  -0.001   0.085   0.083   0.087  -0.005   0.000   0.006   0.144   0.121
OP( 1 &  3 )   0.080   0.004  -0.066   0.034   0.028  -0.072  -0.076  -0.273  -0.411  -0.282
OP( 2 &  3 )   0.005  -0.001   0.008   0.014   0.014  -0.141  -0.137  -0.131  -0.187  -0.171

   Alpha MO:      71      72      73      74      75      76      77      78      79      80
              LUMO+5  LUMO+6  LUMO+7  LUMO+8  LUMO+9 LUMO+10 LUMO+11 LUMO+12 LUMO+13 LUMO+14
 Energy(eV):   -0.08    0.46    0.53    0.56    0.64    0.94    0.97    1.23    1.53    1.61
   Symmetry:     na      na      na      na      na      na      na      na      na      na
==========================================================================================
 FRAG#    1:   33.22   89.99   26.77   35.73    1.02   21.90   26.61    6.94    6.88   11.01
 FRAG#    2:   47.66   -0.84   65.84   57.65   83.75   58.40   61.95    8.27    7.13    8.91
 FRAG#    3:   19.12   10.85    7.39    6.62   15.22   19.70   11.44   84.78   85.99   80.09
OP( 1 &  2 )   0.102  -5.735  -0.506  -1.188  -0.028  -0.251  -0.313  -0.187  -0.453  -2.493
OP( 1 &  3 )  -1.265  -2.917  -0.253  -0.562  -0.024  -0.123  -0.161  -0.075  -0.097   0.262
OP( 2 &  3 )  -0.584   1.057   0.130   0.236   0.075   0.048   0.019  -0.015   0.092  -0.588


Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      3.2814 eV  377.84 nm  f=0.0000  <S**2>=0.000
      64 -> 66         0.10435
      64 -> 67        -0.27280
      65 -> 66         0.57622
      65 -> 68        -0.10468
      65 -> 69         0.11827
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1733.62655260
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      3.3635 eV  368.61 nm  f=0.0003  <S**2>=0.000
      63 -> 66         0.17334
      63 -> 68        -0.20217
      63 -> 70         0.28701
      63 -> 77         0.12136
      64 -> 66        -0.35026
      65 -> 67         0.38605

 Excited State   3:      Singlet-A      3.3715 eV  367.75 nm  f=0.0006  <S**2>=0.000
      63 -> 67         0.17145
      63 -> 69         0.32008
      63 -> 70        -0.11445
      63 -> 76         0.10391
      64 -> 67         0.45597
      64 -> 69         0.15003
      64 -> 70        -0.13439
      65 -> 66         0.23906
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Excited State   4:      Singlet-A      3.4710 eV  357.20 nm  f=0.0005  <S**2>=0.000
      63 -> 66         0.38937
      63 -> 67         0.18898
      63 -> 69         0.22602
      64 -> 66         0.10703
      64 -> 69        -0.16020
      65 -> 66        -0.21116
      65 -> 67        -0.15145
      65 -> 68        -0.15558
      65 -> 69         0.18973
      65 -> 70         0.18783
      65 -> 77         0.10633

 Excited State   5:      Singlet-A      3.4869 eV  355.58 nm  f=0.0008  <S**2>=0.000
      63 -> 66         0.36252
      63 -> 67        -0.19823
      63 -> 68        -0.10601
      63 -> 70         0.14907
      64 -> 66         0.26628
      64 -> 70        -0.16696
      65 -> 66         0.15221
      65 -> 67        -0.19903
      65 -> 68         0.13403
      65 -> 69        -0.18769
      65 -> 70        -0.16025
      65 -> 77        -0.10221

 Excited State   6:      Singlet-A      3.5297 eV  351.26 nm  f=0.0006  <S**2>=0.000
      63 -> 67        -0.33550
      64 -> 67         0.33636
      64 -> 69        -0.32849
      64 -> 76        -0.10621
      65 -> 68        -0.15130
      65 -> 70         0.22968

 Excited State   7:      Singlet-A      3.5393 eV  350.31 nm  f=0.0006  <S**2>=0.000
      63 -> 67        -0.15544
      63 -> 71        -0.13035
      64 -> 66         0.13049
      64 -> 67         0.20857
      64 -> 68        -0.20867
      64 -> 69         0.18149
      64 -> 70         0.26984
      65 -> 69         0.38285
      65 -> 70        -0.21478
      65 -> 76         0.11837

 Excited State   8:      Singlet-A      3.6247 eV  342.05 nm  f=0.0021  <S**2>=0.000
      63 -> 66         0.40084
      63 -> 68         0.17647
      63 -> 69        -0.25412
      63 -> 70        -0.21074
      63 -> 77        -0.15001
      64 -> 66        -0.16972
      64 -> 68        -0.10205
      64 -> 70         0.18993
      64 -> 77         0.10362
      65 -> 67         0.13734
      65 -> 69        -0.13873

 Excited State   9:      Singlet-A      3.6868 eV  336.29 nm  f=0.0015  <S**2>=0.000
      63 -> 67         0.47167
      63 -> 69        -0.22788
      63 -> 70         0.18618
      63 -> 76        -0.11463
      64 -> 67         0.14142
      64 -> 69        -0.23702
      65 -> 68         0.12861
      65 -> 70        -0.14148

 Excited State  10:      Singlet-A      3.9034 eV  317.63 nm  f=0.0001  <S**2>=0.000
      63 -> 68         0.12489
      63 -> 69        -0.23918
      63 -> 70        -0.14510
      64 -> 68         0.23100
      64 -> 70        -0.36353
      65 -> 69         0.38874
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(eta-6-Styrene)Cr(CO)3


 Molecule:    C11H8CrO3
 Details: #P b3lyp/Tzvp SCF=Tight Pop=Full IOp(3/33=1) Guess=Read Geom=Check
 Source file: StyreneB3LYPTzvpAOMix.log
 Population analysis: MPA
  347 orbitals(  347 canonical)  61 alpha +  61 beta electrons
 Number of fragments:    3
 Fragment   1 (  16 atoms,  200 orbitals): Styrene
 Fragment   2 (   6 atoms,  114 orbitals): CO Ligands
 Fragment   3 (   1 atoms,   33 orbitals): Cr

   Alpha MO:      51      52      53      54      55      56      57      58      59      60
              HOMO-10  HOMO-9  HOMO-8  HOMO-7  HOMO-6  HOMO-5  HOMO-4  HOMO-3  HOMO-2  HOMO-1
 Energy(eV):  -10.96  -10.90  -10.87  -10.60  -10.31   -9.56   -9.00   -7.67   -6.03   -5.83
   Symmetry:     na      na      na      na      na      na      na      na      na      na
==========================================================================================
 FRAG#    1:   52.18    6.97   12.81   95.47   98.45   90.95   85.85   90.91    3.06   15.31
 FRAG#    2:   38.51   73.20   69.14    3.77    0.96    2.21    2.22    1.47   24.76   24.29
 FRAG#    3:    9.31   19.83   18.05    0.77    0.59    6.83   11.93    7.62   72.18   60.40
OP( 1 &  2 )  -0.048   0.006   0.005   0.000   0.000  -0.011  -0.001  -0.001   0.007   0.013
OP( 1 &  3 )   0.011  -0.001  -0.004   0.000   0.004   0.050   0.090   0.027  -0.067   0.036
OP( 2 &  3 )   0.061   0.149   0.139   0.005   0.000  -0.001  -0.005   0.000   0.086   0.084

   Alpha MO:      61      62      63      64      65      66      67      68      69      70
                HOMO    LUMO  LUMO+1  LUMO+2  LUMO+3  LUMO+4  LUMO+5  LUMO+6  LUMO+7  LUMO+8
 Energy(eV):   -5.76   -1.85   -1.27   -0.44   -0.40   -0.20    0.03    0.42    0.50    0.51
   Symmetry:     na      na      na      na      na      na      na      na      na      na
==========================================================================================
 FRAG#    1:   18.73   84.56   82.57   17.22   12.56   17.73   62.38   12.06    5.90   10.30
 FRAG#    2:   23.37    8.17   11.88   39.58   46.36   49.67   24.92    2.47   67.33   62.66
 FRAG#    3:   57.91    7.27    5.55   43.21   41.09   32.59   12.70   85.48   26.77   27.03
OP( 1 &  2 )   0.013  -0.076  -0.142  -0.277  -0.239  -0.551  -0.020   0.931   0.088   0.167
OP( 1 &  3 )   0.024  -0.085  -0.077  -0.421  -0.393  -1.056  -0.238  -2.471  -0.096  -0.340
OP( 2 &  3 )   0.082   0.026   0.001   0.108   0.157   0.087  -0.253  -5.174  -0.383  -0.759

Excitation energies and oscillator strengths:

 Excited State   1:      Singlet-A      2.9053 eV  426.75 nm  f=0.0010  <S**2>=0.000
      60 -> 62         0.68708
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1694.31620642
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      3.0587 eV  405.35 nm  f=0.0045  <S**2>=0.000
      59 -> 62         0.60470
      59 -> 65        -0.14113
      60 -> 63         0.13598
      61 -> 62         0.25997

 Excited State   3:      Singlet-A      3.1145 eV  398.09 nm  f=0.0296  <S**2>=0.000
      59 -> 62        -0.30536
      60 -> 63         0.27159
      61 -> 62         0.53484
      61 -> 64        -0.11349

 Excited State   4:      Singlet-A      3.3052 eV  375.12 nm  f=0.0001  <S**2>=0.000
      59 -> 64        -0.22044
      60 -> 63         0.14604
      60 -> 64         0.10627
      61 -> 63         0.58314
      61 -> 64         0.16741
      61 -> 65         0.10826

 Excited State   5:      Singlet-A      3.4452 eV  359.87 nm  f=0.0008  <S**2>=0.000
      59 -> 63         0.42045
      59 -> 64         0.40944
      59 -> 69        -0.10884
      59 -> 73         0.10863
      60 -> 64         0.11139
      60 -> 65        -0.16243
      61 -> 63         0.17437
      61 -> 65         0.10736
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Excited State   6:      Singlet-A      3.4625 eV  358.08 nm  f=0.0010  <S**2>=0.000
     59 -> 63        -0.11737
     59 -> 65        -0.27126
     60 -> 63         0.10561
     60 -> 64         0.36947
     60 -> 65        -0.23310
     61 -> 63        -0.22081
     61 -> 64         0.28834
     61 -> 65         0.14274

Excited State   7:      Singlet-A      3.5343 eV  350.80 nm  f=0.0006  <S**2>=0.000
     59 -> 65         0.17474
     59 -> 66         0.13512
     60 -> 64         0.25856
     60 -> 65         0.23351
     61 -> 64        -0.25968
     61 -> 65         0.42173

Excited State   8:      Singlet-A      3.5560 eV  348.67 nm  f=0.0032  <S**2>=0.000
     59 -> 63         0.16564
     59 -> 64        -0.15708
     59 -> 65         0.36654
     59 -> 70         0.10249
     59 -> 74         0.10652
     60 -> 64        -0.14267
     60 -> 65        -0.18440
     61 -> 62         0.11514
     61 -> 63        -0.20639
     61 -> 64         0.30638
     61 -> 65         0.13922
     61 -> 72        -0.11738

Excited State   9:      Singlet-A      3.6396 eV  340.65 nm  f=0.0014  <S**2>=0.000
     59 -> 63         0.49989
     59 -> 64        -0.25657
     59 -> 65        -0.17466
     59 -> 72         0.10731
     60 -> 65         0.25381
     60 -> 72        -0.10337
     61 -> 64         0.10447

Excited State  10:      Singlet-A      3.8885 eV  318.85 nm  f=0.0029  <S**2>=0.000
     59 -> 64         0.28325
     60 -> 63         0.12926
     60 -> 64        -0.23060
     60 -> 65         0.37417
     61 -> 64         0.32438
     61 -> 65         0.17671
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Kinetic Analyses

Kinetic Analysis of (eta-6-benzophenone)Cr(CO)3 Transient signals

470 nm excitation

1965 Band Single Expontential Curve Fitting

		Value	Standard Error
1965	y0	-4.19763E-4	4.81883E-5
1965	A1	-0.00206	5.47435E-5
1965	t1	-1.27178E-11	1.07136E-12

Number of Points	86
Degrees of Freedom	83
Reduced Chi-Sqr	2.18542E-8
Residual Sum of Squares	1.8139E-6
Adj. R-Square	0.94388
Fit Status	Succeeded(100)

2008 Band Single Exponential Curve Fitting

		Value	Standard Error
2008	y0	1.28339E-4	1.39461E-5
2008	A1	0.00132	3.60763E-5
2008	t1	6.77533E-12	3.51052E-13

Number of Points	86
Degrees of Freedom	83
Reduced Chi-Sqr	4.94448E-9
Residual Sum of Squares	4.10392E-7
Adj. R-Square	0.96038
Fit Status	Succeeded(100)

320 nm Excitation

1843 Single Exponential Curve Fitting

		Value	Standard Error
1843	y0	6.38375E-4	6.15733E-6
1843	A1	-3.37668E-4	7.32654E-6
1843	t1	-5.18538E-11	3.04456E-12

Number of Points	69
Degrees of Freedom	66
Reduced Chi-Sqr	2.774E-10
Residual Sum of Squares	1.83084E-8
Adj. R-Square	0.96918
Fit Status	Succeeded(100)

Kinetic Analysis of (eta-6-Styrene)Cr(CO)3 Transient signals

400 nm Excitation

Grow-in of reactive excited state

1966 Single Exponential Curve Fitting

		Value	Standard Error
1966	y0	0.00171	1.00045E-4
1966	A1	-0.00182	1.14507E-4
1966	t1	-2.01035E-12	3.59568E-13

Number of Points	9
Degrees of Freedom	6
Reduced Chi-Sqr	6.06619E-9
Residual Sum of Squares	3.63972E-8

Adj. R-Square 0.96969
Fit Status Succeeded(100)

Recovery of Parent Absorbances

1983 Band

		Value	Standard Error
1983	y0	-0.00297	4.27297E-5
1983	A1	-0.00495	1.13001E-4
1983	t1	-2.57462E-11	1.08249E-12

Number of Points 17
Degrees of Freedom 14
Reduced Chi-Sqr 6.03311E-9
Residual Sum of Squares 8.44636E-8
Adj. R-Square 0.99541
Fit Status Succeeded(100)

Decay of Reactive Excited State

1966 Band

		Value	Standard Error
1966	y0	-1.34211E-4	1.67078E-5
1966	A1	0.00209	1.96177E-5
1966	t1	4.98648E-11	1.2656E-12

Number of Points 17
Degrees of Freedom 14
Reduced Chi-Sqr 4.19734E-10
Residual Sum of Squares 5.87627E-9
Adj. R-Square 0.99861
Fit Status Succeeded(100)

Kinetic Analysis of (eta-6-Allylbenzene)Cr(CO)3 Transient signals

400 nm Excitation

Grow-in of reactive excited state

1958 Band

		Value	Standard Error
1958	y0	9.15279E-4	3.33429E-5
1958	A1	-0.00129	7.9541E-5
1958	t1	-1.30047E-12	1.61119E-13

1958
Number of Points 9
Degrees of Freedom 6
Reduced Chi-Sqr 1.60132E-9
Residual Sum of Squares 9.60791E-9
Adj. R-Square 0.98122
Fit Status Succeeded(100)

Decay of Reactive Excited State

1958 Band

		Value	Standard Error
1958	y0	-1.91262E-5	7.83047E-6
1958	A1	0.00113	1.22143E-5
1958	t1	4.24781E-11	1.09932E-12

Number of Points 16
Degrees of Freedom 13
Reduced Chi-Sqr 1.10589E-10
Residual Sum of Squares 1.43765E-9
Adj. R-Square 0.99855
Fit Status Succeeded(100)

Grow-in of CO-loss

1918 Band

		Value	Standard Error
1918	y0	0.00114	1.71716E-5
1918	A1	-0.00131	3.23346E-5
1918	t1	-3.70118E-11	1.97781E-12

Number of Points	16	
Degrees of Freedom	13	
Reduced Chi-Sqr		6.28767E-10
Residual Sum of Squares		8.17397E-9
Adj. R-Square	0.99359	
Fit Status	Succeeded(100)	

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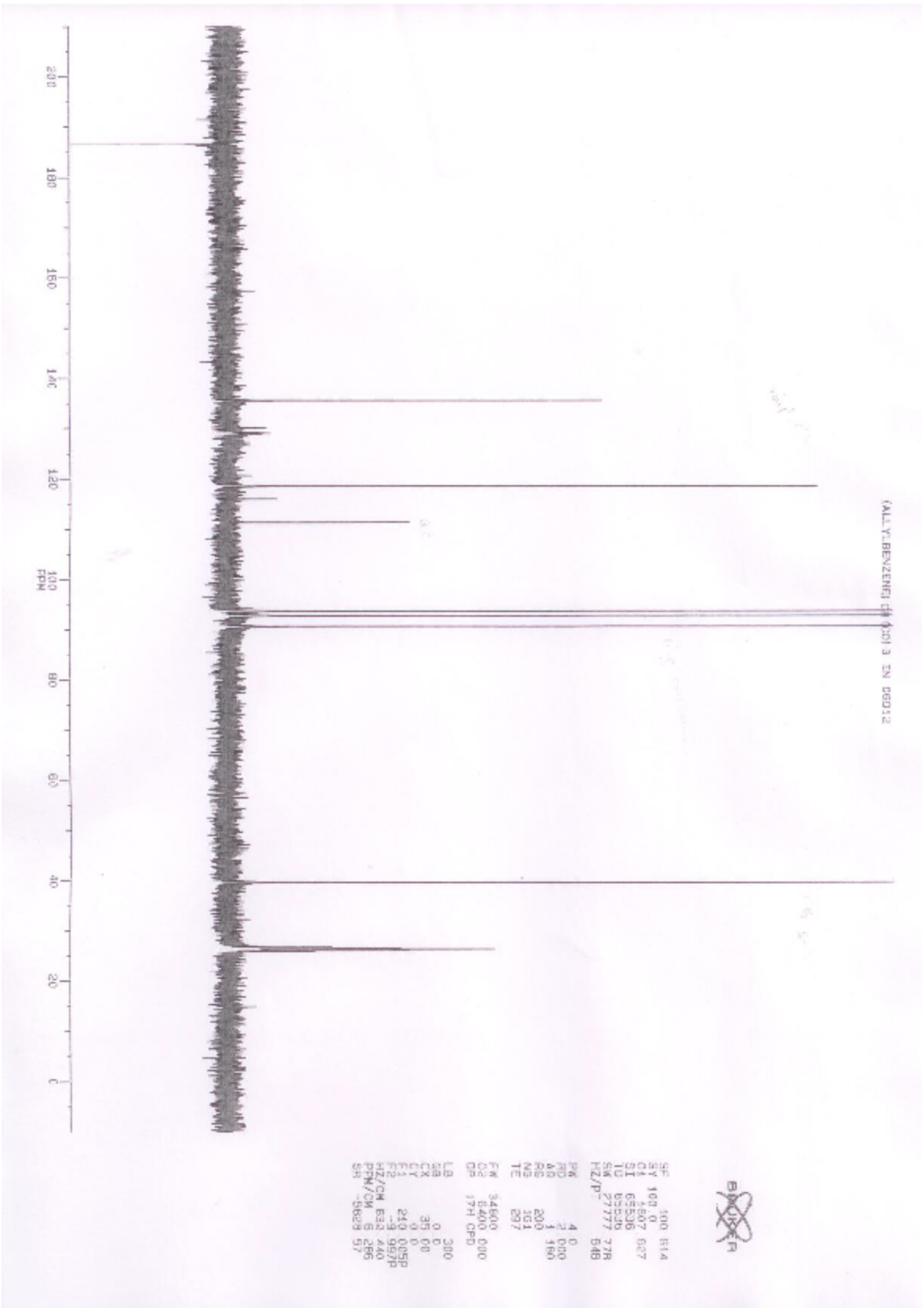
(η^6-Allylbenzene)$Cr(CO)_3$ Analytical Data ^{13}C nmr in C_6D_{12}



(η^6-Allylbenzene)Cr(CO)$_3$ Analytical Data Mass Spectrum